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Energy dissipation in granular materials in triaxial tests

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ABSTRACT

The triaxial test is used in a laboratory to investigate the behaviour of geotechnical materials (e.g. clays and sands). The difficulty in measuring some properties of granular media such as energy changes throughout the test have motivated the current numerical simulations of this test. This paper presents a description of a series of triaxial tests using LIGGGHTS open source Discrete Element Modelling software in a study of how energy is dissipated in granular media. The simulated triaxial tests are being carried out on cube shaped samples with six mesh walls enclosing the particles. Three of the walls (i.e. bottom, left and back walls) are fixed in position while the other three walls are allowed to move. Energy dissipation will be investigated by tracing changes of the energy terms at various time steps and applying the principle of energy conservation. The relationship between confining pressure, particle size distribution, friction coefficient and the voids ratio with energy dissipation will be investigated during the analysis of the results from the simulations. It is hoped that understanding the relationship between grain scale parameters and energy dissipation will help in the formulation of constitutive relationships within, for instance, the hyperplasticity framework. It is envisioned that relating grain scale parameters to constitutive models will allow the formulation of models that are purely based on the micro mechanics of granular media.

Key Words: *DEM; energy dissipation; compression; triaxial test; hyperplasticity*

1. Introduction

The Discrete Element Method (DEM) introduced by Cundall and Strack [1] has been used in numerous numerical modelling studies over the past few decades. It models individual particles by considering the laws of motion. In civil engineering, it has been used to study geotechnical materials (mainly sands). DEM modelling is a numerical tool that is able to capture physically difficult to measure details about granular media such as particle rotations, displacements and energy evolutions. As such, it has been used to model geotechnical laboratory tests (e.g. direct shear and triaxial tests), and used them to study the behaviour of granular media closely. Examples of such modelling can be found in [2] and [11]. This paper focuses on the simulation of triaxial tests to study energy dissipation in granular media.

Energy dissipation in granular media has been a subject of interest in recent years. The relationship between energy dissipation and particle crushability, grain roughness, and energy dissipation response to seismic loading are some examples of many studies on energy dissipation in granular media [10, 6, 9]. Mukwiri et al. [7] recently highlighted an area of research in which grain scale parameters could potentially be linked to constitutive models by gaining a deeper understanding of energy dissipation in granular media. The simulations presented in this paper will hopefully build on that work by using triaxial tests to obtain relationships between grain scale parameters and energy dissipation.

2. Numerical simulations

The triaxial tests are being carried out using an open source DEM particle simulation software, LIGGGHTS developed by Kloss et al. [5]. Unlike the commercial DEM software, LIGGGHTS has no user interface. Simulations are driven using text-based input scripts containing series of commands to conduct the simulation.

The scripts that drive the simulations for the present study could be broken down into four parts: initialisation, setup, general settings, and execution. In the initialisation part, the simulation geometry is specified and set to be of moving boundaries to allow the sample to move outward during the simulation. Any required memory settings are also set in this part. Within the setup part, the material properties of the particles that would be inserted are declared. The simulation procedures are also stated in this part. The general settings part of the scripts is where settings that corresponded to speed and memory utilisation are specified and the output options also generated. Each script is then supplied with execution commands to be carried out at various stages of the simulation. Throughout the simulations, files are output for later post processing.

The triaxial test simulations model spherical particles each of density 2650 kg/m^3, Poisson's ratio of 0.25, and Young's modulus of 70 GPa. Each simulation sample size is a cube of 0.1 m length. With these details, the simulations are set up such that three enclosing walls (i.e. top, right and front walls) would be allowed to move while the rest are be fixed. The walls allowed to move are inserted into the sample as servo walls and set to compress the particles until a target total force corresponding to a desired pressure on the wall is achieved.

For each triaxial test, the particles are inserted at half the target particle diameter and then grown in size. This is done to speed up the particle insertion stage of the simulation. Once this stage is completed, the particles are then allowed to settle before the consolidation stage. A hydrostatic confining pressure (σ) is then applied to the servo walls during consolidation. Front and right walls are then maintained at this pressure and the top wall is allowed to move at a maximum set velocity of 0.001 m/s downwards during shearing. To ensure that the desired pressure is accurate, the target total force on the walls is updated at every time step by evaluating the product of σ and the current wall contact area with the particles.

Four parameters will be varied during this study: the confining pressure (σ), particle-particle friction coefficient (μ), initial voids ratio before consolidation (e_{ini}), and the coefficient of uniformity (C_u). The particle-wall coefficient of friction for each simulation is kept at zero. C_u is a particle size distribution measurement given by

$$C_u = \frac{d_{60}}{d_{10}} \tag{1}$$

where d_{60}, d_{30}, and d_{10} are equivalent to grading sieve sizes used in a laboratory to determine the particle size distribution of soils. 60, 30 and 10 values are the percentage of particles that go through the sieve size considered. These d values correspond to particle diameters when modelled using DEM.

Table 1: Simulation for the triaxial tests

Parameter/No.	1	2	2	4	5	6	7	8	9
σ (kPa)	100	100	100	400	400	400	800	800	800
μ	0.2	0.3	0.5	0.2	0.3	0.5	0.2	0.3	0.5
C_u	1	3	6	3	6	1	6	1	3
e_{ini}	0.4	0.6	0.8	0.8	0.4	0.6	0.6	0.8	0.4

The intended number of simulations to run was obtained using the Taguchi experimental design technique [8]. This analysis involves defining a suitable orthogonal two dimensional array matrix that defines all the variable settings required for each experiment. The technique helped to reduce the number of simulations that would be required to vary all four variable parameters in this study at three levels each. If one parameter would be changed at a time, 81 simulations would have been required. However, using the Taguchi method reduced this number to nine simulations shown in Table 1. The meaning of orthogonality in this context is "statical independence" [8]. In Table 1, each row has each level of a parameter appearing an equal number of times. Further more, statical independence also means that the relationship between one row and another is such that each each level in any other row will occur an equal number of times as well.

3. Energy monitoring

To facilitate the study of energy dissipation for the triaxial tests, energy monitoring is done by post processing the files output during the simulations. This process is done using Matlab. The energy equation used is

$$dE_p + dW = dE_k + dE_\mu + dE_\zeta + dU, \tag{2}$$

where dE_p is the change in potential energy, dW the change in boundary work, dE_k the change in kinetic energy, dE_μ is the dissipated frictional energy, dE_ζ the change in dissipated energy through damping, and dU is the change in stored work.

The total change in dissipated energy, dE_η during the simulations comes from the dE_μ and the dE_ζ terms of (2). Since the simulations are pseudo static, it was found that the potential and kinetic energies are each $\approx 10^6$ times smaller than either of the boundary work or the stored elastic energy. We can therefore re-write (2) as

$$dE_\eta \approxeq dW - dU \tag{3}$$

The change in boundary work is calculated as:

$$dW = \sum_{j=1}^{m} \sigma_v^j A_S^j \delta x^j, \tag{4}$$

where σ_v is the normal stress on mesh j, which is the sum of all the individual stress values from each triangular mesh element, i composing it. A_S is the surface area of the mesh considered and is obtained by summing up the areas of each triangular mesh element, i as

$$A_S = \frac{1}{2}\sum_{i=1}^{n} |\mathbf{AB}_i \times \mathbf{AC}_i|, \tag{5}$$

where the area of each triangular element with vertices A, B and C is calculated using cross product between vectors **AB** and **AC**.

Changes in the stored energy are due to the evolution of normal and tangential contact forces. The summation of strain energy for all the contacts is equal to the stored energy, dU and is calculated as

$$dU = dU^n + dU^t, \tag{6}$$

where dU^n and dU^t are the contributions from normal and tangential contact forces and are equal to

$$dU^n = \int_0^{\delta_n} \underbrace{\overbrace{\frac{4}{3}E^*\sqrt{R^*\delta_n}}^{K_n}\,\delta_n\mathbf{n}}_{F^n}\, d_n \tag{7}$$

and

$$dU^t = \int_0^{\xi_t} \underbrace{\overbrace{8G^*\sqrt{R^*\delta_n}}^{K_t}\,\xi_t}_{F^t}\, d\xi_t, \tag{8}$$

respectively. F^n and F^t are in turn the normal and tangential contact forces and K_n and K_t are the corresponding stiffness parameters from the Hertzian contact model, which governs how spherical particles interact at contact. Two particles 1 and 2 will have an effective radius, $R^* = R_1R_2/(R_1 + R_2)$, which is the geometric mean of radii R_1 and R_2. $\delta_n = R_1 + R_2 - d_{12}$ and is the overlap at contact between the two particles in the normal direction where d_{12} is the distance between their centres. The effective Young's modulus, $E^* = 0.5E/(1 - \nu^2)$, is derived from the particles' material Young's modulus, E and Poisson's ratio, ν. In Equation (7), $\boldsymbol{n}$ is the normal vector for the particles in contact. The term $\boldsymbol{\xi_t}$ in Equation (8) is the tangential displacement and is calculated by integrating the tangential relative velocity over the contact time [3].

4. Further analysis

Sections 2 and 3 have described the simulations procedures and the method used to post process for energy dissipation. Currently, these simulations are being done and the results will be used to investigate the relationship between grain scale parameters and energy dissipation in triaxial tests. The influence of particle size distribution, initial voids ratio, friction coefficients, and the confining pressure will in particular be studied. The present plan is to only have the nine simulations described in Section 2, however, more simulations can be conducted if required.

It is hoped that the observations made from this analysis will facilitate the development of energy dissipation functions that are purely based on grain scale parameters.

The energy dissipation functions formed would then be used to formulate yield surfaces and plastic flow rules which would describe the inelastic behaviour of these materials (sands in particular) based on the hyperplasticity framework [4]. This would potentially facilitate the formation of constitutive models informed by grain scale parameters. This method of formulating constitutive models could then be further extended to all granular media.

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